

## Uploading L5.str



```

chain nodes :
16 17 18 19 24 25 26 31 37 38 39 40 41 42 43 44 49 50 54 55 57
58 59 60 61 62 66 67 68 69 74 75 76 78
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 30 32 36
chain bonds :
1-78 11-69 12-68 13-67 14-66 24-25 30-31 31-54 32-55 36-39 36-41 37-40
37-42 38-43 38-44 57-74 58-75 58-76 59-60
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 4-10 5-6 7-8 8-9 9-10 9-11 10-14 11-12 12-13
13-14
exact/norm bonds :
1-2 1-6 1-78 2-3 3-4 4-5 4-7 4-10 5-6 7-8 8-9 11-69 12-68 13-67 14-66
24-25 30-31 31-54 32-55 36-39 36-41 37-40 37-42 38-43 38-44 57-74 58-75
58-76 59-60

normalized bonds :
9-10 9-11 10-14 11-12 12-13 13-14

```

G2: [\*1], [\*2]

G3: [\*3], [\*4]

G4: [\*5], [\*6], [\*7]

G6: [\*8], [\*9], [\*10], [\*11]

G8: H, CN, X, Ak

G9: [\*12], [\*13], [\*14]

G10: [\*15], [\*16], [\*17], [\*18]

```
Connectivity :  
2:2 E exact RC ring/chain 6:2 E exact RC ring/chain 50:1 E exact RC ring/chain  
57:2 E exact RC ring/chain  
Match level :
```

10/517,957

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS 24:CLASS  
25:CLASS 26:CLASS  
30:Atom 31:CLASS 32:Atom 36:Atom 37:CLASS 38:CLASS 39:CLASS 40:CLASS  
41:CLASS 42:CLASS  
43:CLASS 44:CLASS 49:CLASS 50:CLASS 54:CLASS 55:CLASS 57:CLASS 58:CLASS  
59:CLASS 60:CLASS  
61:CLASS 62:Atom 66:CLASS 67:CLASS 68:CLASS 69:CLASS 74:CLASS 75:CLASS  
76:CLASS 78:CLASS

Generic attributes :

62:  
Saturation : Unsaturat

=> d his full

(FILE 'HOME' ENTERED AT 15:28:30 ON 04 AUG 2008)

FILE 'REGISTRY' ENTERED AT 15:33:17 ON 04 AUG 2008

L1 STRUCTURE uploaded  
D L1  
L2 50 SEA SSS SAM L1  
L3 STRUCTURE uploaded  
D L3  
L4 50 SEA SSS SAM L3  
L5 STRUCTURE uploaded  
L6 48 SEA SSS SAM L5  
D STAT QUERY  
L7 1778 SEA SSS FUL L5  
SAVE TEMP L7 SZN957L7ST/A  
SAVE TEMP L7 SZN957L5ST/A

FILE 'HCAPLUS' ENTERED AT 16:34:53 ON 04 AUG 2008

L8 57 SEA ABB=ON PLU=ON L7  
D OCC L8 1-57  
L9 ANALYZE PLU=ON L8 1- RN HIT : 618 TERMS

FILE 'REGISTRY' ENTERED AT 16:38:59 ON 04 AUG 2008

L10 ANALYZE PLU=ON L7 1- LC : 8 TERMS  
D  
L11 1160 SEA ABB=ON PLU=ON L7 NOT CAPLUS/LC  
D IDE 1  
D IDE 1160  
D COST  
D ALL 1160  
D COST  
L12 1150 SEA ABB=ON PLU=ON L11 AND ED<20030604  
L13 0 SEA ABB=ON PLU=ON L11 AND AMBINTER?/SR,SO

FILE 'STNGUIDE' ENTERED AT 16:50:43 ON 04 AUG 2008

FILE 'REGISTRY' ENTERED AT 16:51:41 ON 04 AUG 2008  
E A/SR

L14 1150 SEA ABB=ON PLU=ON L11 AND (CHEMICAL LIB?/SR)  
L15 10 SEA ABB=ON PLU=ON L11 NOT L14

D IDE L15 1  
 D IDE L15 10  
 L16 0 SEA ABB=ON PLU=ON L12 AND AMBINTER?/ENTE  
 L17 618 SEA ABB=ON PLU=ON L7 AND CAPLUS/LC  
 L18 5380072 SEA ABB=ON PLU=ON CASREACT/LC  
 L19 62694 SEA ABB=ON PLU=ON L18 NOT CAPLUS/LC  
 L20 ANALYZE PLU=ON L12 1- SR : 1 TERM  
 D

FILE 'REGISTRY' ENTERED AT 17:17:15 ON 04 AUG 2008  
 D STAT QUERY L12  
 D L12 IDE 1,101,201,301,401,501,601,701,801,901,1001,1101

FILE 'HCAPLUS' ENTERED AT 17:21:12 ON 04 AUG 2008  
 E HUGHES D?/AU  
 L21 2265 SEA ABB=ON PLU=ON HUGHES D?/AU  
 E WORTHINGTON P?/AU  
 L22 178 SEA ABB=ON PLU=ON WORTHINGTON P?/AU  
 E RUSSEL C?/AU  
 L23 133 SEA ABB=ON PLU=ON RUSSEL C?/AU  
 E CLARKE E?/AU  
 L24 471 SEA ABB=ON PLU=ON CLARKE E?/AU  
 E PEACE J?/AU  
 L25 57 SEA ABB=ON PLU=ON PEACE J?/AU  
 E ASHTON M?/AU  
 E COULTER T?/AU  
 L26 49 SEA ABB=ON PLU=ON COULTER T?/AU  
 E ROBERTS R?/AU  
 L27 3528 SEA ABB=ON PLU=ON ROBERTS R?/AU  
 E MOLLEYRES L?/AU  
 L28 31 SEA ABB=ON PLU=ON MOLLEYRES L?/AU  
 E CEDERBAUM F?/AU  
 L29 43 SEA ABB=ON PLU=ON CEDERBAUM F?/AU  
 E ASHTON M?/AU  
 L30 168 SEA ABB=ON PLU=ON ASHTON M?/AU  
 L31 0 SEA ABB=ON PLU=ON L21 AND L22 AND L23 AND L24 AND L25 AND  
 L26 AND L27 AND L28 AND L29 AND L30  
 L32 18 SEA ABB=ON PLU=ON L21 AND ((L22 OR L23 OR L24 OR L25 OR L26  
 OR L27 OR L28 OR L29 OR L30))  
 L33 2 SEA ABB=ON PLU=ON L22 AND (L23 OR L24 OR L25 OR L26 OR L27  
 OR L28 OR L29 OR L30)  
 L34 0 SEA ABB=ON PLU=ON L23 AND (L24 OR L25 OR L26 OR L27 OR L28  
 OR L29 OR L30)  
 L35 1 SEA ABB=ON PLU=ON L24 AND (L25 OR L26 OR L27 OR L28 OR L29  
 OR L30)  
 L36 1 SEA ABB=ON PLU=ON L25 AND ((L26 OR L27 OR L28 OR L29 OR  
 L30))  
 L37 2 SEA ABB=ON PLU=ON L26 AND (L27 OR L28 OR L29 OR L30)  
 L38 1 SEA ABB=ON PLU=ON L27 AND (L28 OR L29 OR L30)  
 L39 1 SEA ABB=ON PLU=ON L29 AND L30  
 E CASSAYRE J?/AU  
 L40 31 SEA ABB=ON PLU=ON CASSAYRE J?/AU  
 E MAIENFISCH P?/AU  
 L41 113 SEA ABB=ON PLU=ON MAIENFISCH P?/AU  
 L42 0 SEA ABB=ON PLU=ON L21 AND L22 AND L23 AND L24 AND L25 AND  
 L26 AND L27 AND L28 AND L29 AND L30 AND L40 AND L41  
 L43 18 SEA ABB=ON PLU=ON L21 AND ((L22 OR L23 OR L24 OR L25 OR L26  
 OR L27 OR L28 OR L29 OR L30) OR L40 OR L41)  
 L44 2 SEA ABB=ON PLU=ON L22 AND ((L23 OR L24 OR L25 OR L26 OR L27  
 OR L28 OR L29 OR L30) OR L40 OR L41)

L45 0 SEA ABB=ON PLU=ON L23 AND ((L24 OR L25 OR L26 OR L27 OR L28  
OR L29 OR L30) OR L40 OR L41)  
L46 1 SEA ABB=ON PLU=ON L24 AND ((L25 OR L26 OR L27 OR L28 OR L29  
OR L30) OR L40 OR L41)  
L47 1 SEA ABB=ON PLU=ON L25 AND ((L26 OR L27 OR L28 OR L29 OR L30)  
OR L40 OR L41)  
L48 2 SEA ABB=ON PLU=ON L26 AND ((L27 OR L28 OR L29 OR L30) OR L40  
OR L41)  
L49 1 SEA ABB=ON PLU=ON L27 AND ((L28 OR L29 OR L30) OR L40 OR  
L41)  
L50 11 SEA ABB=ON PLU=ON L28 AND ((L29 OR L30) OR L40 OR L41)  
L51 13 SEA ABB=ON PLU=ON L29 AND (L30 OR L40 OR L41)  
L52 1 SEA ABB=ON PLU=ON L30 AND (L40 OR L41)  
L53 18 SEA ABB=ON PLU=ON L40 AND L41  
L54 40 SEA ABB=ON PLU=ON (L42 OR L43 OR L44 OR L45 OR L46 OR L47 OR  
L48 OR L49 OR L50 OR L51 OR L52 OR L53)  
L55 6999 SEA ABB=ON PLU=ON (L21 OR L22 OR L23 OR L24 OR L25 OR L26 OR  
L27 OR L28 OR L29 OR L30) OR L40 OR L41  
L56 117 SEA ABB=ON PLU=ON L55 AND SYNGENTA?/CO,CS,PA,SO  
L57 35 SEA ABB=ON PLU=ON L54 AND SYNGENTA?/CO,CS,PA,SO  
L58 68 SEA ABB=ON PLU=ON L56 AND (PEST? OR INSECT? OR ACARI? OR  
MITE OR MITIC? OR NEMAT? OR MOLLUSC?)  
L59 32 SEA ABB=ON PLU=ON L57 AND (PEST? OR INSECT? OR ACARI? OR  
MITE OR MITIC? OR NEMAT? OR MOLLUSC?)  
L60 7 SEA ABB=ON PLU=ON L58 AND (SPIRO? OR INDOLIN? OR SPIROINDOLIN  
?)  
L61 32 SEA ABB=ON PLU=ON L59 OR L60  
L62 4 SEA ABB=ON PLU=ON L58 AND ((CROP OR PLANT) (6A) (PROTECT? OR  
CHEMIC?))  
L63 36 SEA ABB=ON PLU=ON L61 OR L62  
L64 10 SEA ABB=ON PLU=ON L58 AND ?PIPERIDIN?  
L65 37 SEA ABB=ON PLU=ON L64 OR L63  
SAVE TEMP L65 SZN957HCIN/A  
D STAT QUERY L8  
D L8 1-57 IBIB ED ABS HITSTR  
D QUE L65  
D L65 1-37 IBIB ABS

FILE 'MEDLINE, BIOSIS, EMBASE, AGRICOLA' ENTERED AT 17:51:30 ON 04 AUG  
2008

L66 11 SEA ABB=ON PLU=ON L65  
D L66 1-11 AU  
D QUE L66

FILE 'HCAPLUS, MEDLINE, BIOSIS, EMBASE' ENTERED AT 17:54:07 ON 04 AUG 2008

L67 46 DUP REM L65 L66 (2 DUPLICATES REMOVED)  
ANSWERS '1-37' FROM FILE HCAPLUS  
ANSWERS '38-39' FROM FILE MEDLINE  
ANSWERS '40-46' FROM FILE BIOSIS  
D L67 38-46 IBIB AB

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 2 AUG 2008 HIGHEST RN 1037774-47-2  
DICTIONARY FILE UPDATES: 2 AUG 2008 HIGHEST RN 1037774-47-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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FILE HCPLUS

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FILE COVERS 1907 - 4 Aug 2008 VOL 149 ISS 6

FILE LAST UPDATED: 3 Aug 2008 (20080803/ED)

HCplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Aug 1, 2008 (20080801/UP).

FILE MEDLINE

FILE LAST UPDATED: 3 Aug 2008 (20080803/UP). FILE COVERS 1949 TO DATE.

MEDLINE has been updated with the National Library of Medicine's revised 2008 MeSH terms. See HELP RLOAD for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

See HELP RANGE before carrying out any RANGE search.

FILE BIOSIS

FILE COVERS 1926 TO DATE.

CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT FROM JANUARY 1926 TO DATE.

RECORDS LAST ADDED: 31 July 2008 (20080731/ED)

10/517,957

BIOSIS has been augmented with 1.8 million archival records from 1926 through 1968. These records have been re-indexed to match current BIOSIS indexing.

FILE EMBASE

FILE COVERS 1974 TO 4 Aug 2008 (20080804/ED)

EMBASE was reloaded on March 30, 2008.

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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FILE AGRICOLA

FILE COVERS 1970 TO 8 Jul 2008 (20080708/ED)

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